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We proposed to study several different types of problems involving partial differential equations which arise naturally in applications: (1) Qualitative behavior of solutions of nonlinear evolution equations. (2) Parameter identification problems.

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Final Technical Report
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(October 1, 1988 - September 30, 1989)

by

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Table of Contents

I. Summary.

We proposed to study several different types of problems involving partial differential equations which arise naturally in applications.

1. **Qualitative behavior of solutions of nonlinear evolution equations**. We considered certain scalar nonlinear hyperbolic and parabolic equations, and also parabolic systems arising in chemical reaction kinetics. We wanted, first of all, to locate certain special kinds of solutions when they exist, for example equilibrium states, traveling waves, and time periodic solutions, or in some cases co-called breather solutions (spatially localized time periodic solutions). Also we investigated the large time behavior of solutions of the evolution problem with particular attention to the behavior of solutions which are close to the special form solutions mentioned above. That is to say, the stability properties of equilibrium states, periodic solutions, etc. will be studied. In some cases blow up of solutions may occur (in which case there is no large time behavior) and in this situation we wanted to understand as much as possible which solutions blew up, the nature of the blow up, and which solutions existed for all times.

2. **Parameter identification problems**. Basic questions of seismic exploration and other types of remote sensing problems lead naturally to problems of determining coefficients in a linear hyperbolic equation or system, using as data some limited knowledge of special solutions of the differential equation. That is to say, we try to infer knowledge about the internal structure of a wave propagating medium by observing how it responds to some stimulus.

Also in this category are problems of determining the dependence of solutions on parameters in the problem. The partial differential equations often come to us from physical models containing one or more parameters: Reynolds number, reaction rates, diffusivities, etc. An important problem is deciding for which values of the parameters solutions of certain special form exist, and what is the effect on the evolution problem when the parameters are varied in some way. Mathematically we are lead to nonlinear eigenvalue problems, bifurcation problems, etc.

There are serious computational issues associated with many of the above questions. Indeed, in the case of coefficient identification problems it is always a central concern to develop useful solution algorithms. In the case of the equations of chemical reaction kinetics when there may be very complicated dependence of solutions on many parameters, it may be that computational continuation methods are the most reasonable way of studying, for example, a branch of periodic solutions emanating from a Hopf bifurcation point. Even in those situations when the numerical solutions are not of primary interest, numerical experiments will be of great help in guiding theoretical investigations.

II. Research Objectives.

(Levine)

1. Nonlocal parabolic equations. We are continuing our investigation into the long time behavior of solutions of nonlocal reaction diffusion equations of the form

$$u_t = u_{xx} + \varepsilon u u_x + a\left(\|u\|^{p-1} + b\right) \cdot u \tag{1}$$

where $\| \quad \|$ denotes the L_1 norm (in x) and where a, b are constants. This equation was studied numerically by Djomeri, Ewing, Jacobs and Straughan in their article *"Nonlinear instability for a modified form of Burger' equation"* which appeared in Numerical Methods for Partial Differential equations 3(1987). It was proposed by Drazin and Reid (Hydrodynamic Stability, Cambridge University Press) as a model for hydrodynamic flows with nonlinear effects.

We have obtained a rather complete theoretical picture of the set of stationary solutions for (1) under Dirichlet boundary conditions as well as an analysis of solutions whose initial values are small perturbations of stationary solutions. We have begun to prepare the report on this work.

2. Reaction-Diffusion equations. In our recent work with Bandle (*"On the Existence and Nonexistence of Global Solutions to Reaction Diffusion Equations in Sectorial Domains"* which has been accepted for publication in the Transactions of the American Mathematical Society), we studied the equation (with Dirichlet boundary conditions)

$$\begin{aligned} u_t &= \Delta u + u^p \qquad \text{in} \quad D \times (0,T) \\ u &= 0 \qquad\qquad\quad \text{on} \quad \partial D \times (0,T) \end{aligned} \tag{2}$$

which is often used to model chemically reacting systems. We showed that if the space domain was a cone then there were two numbers $\underline{p}$ and $\bar{p}$ such that if $1 < p < \underline{p}$ then no nonnegative nontrivial global solution of (2) is possible, while if $p > \bar{p}$, then there are positive global solutions. A similar result was proved for (2) in the case that D was the exterior of a bounded region. (They also took up the question of the existence of stationary solutions and showed that under the condition that $1 < p \leq \bar{p}$ then there were none and that if $p > \bar{p}$ then they could not decay rapidly at infinity).

P. Meier, a former student of Bandle, and Levine have recently sharpened the above result to show that if $p > \underline{p}$ then again nontrivial positive solutions do exist for all time. To do this is was necessary to construct a super solution that did not involve the Green's function as did the earlier argument of Fujita in the case that the domain was all of space.

3. Quenching of solutions of singular equations. We have continued our study of the long time behavior of

$$u_t = \Delta u + \varepsilon(1-u)^{-\beta} \tag{3}$$

on space-time cylinders with a bounded spatial domain. In the case of one space dimension, we have obtained a complete picture of the dynamical behavior of solutions. Deng (a Ph.D. student of Levine) and Levine have also shown that (in any space dimension) the set of points where the solution quenches is contained in a compact subdomain of the (convex) space domain and that on this set the time derivative blows up. This result uses some modifications of some recent results of Friedman and McLeod. It considerably improves a recent result of Acker and Kawohl who proved the blow up of u_t at quenching when the space domain is a ball and the initial data is radially decreasing. We only require that $u_t(x,0)$ be nonnegative.

4. We have begun to look at the following system with Payne and Straughan.

$$
\begin{array}{lll}
u_t + v u_x = u_{xx} + \theta + u^2 & x > 0, & t > 0 \\
\theta_t + v\theta_x = \nu \cdot \theta_{xx} & x > 0, & t > 0 \\
u = v_x & x > 0, & t > 0 \\
v(0,t) = u(0,t) = 0 & t \geq 0 & \\
v(\infty,t) = \theta(\infty,t) = 0 & t \geq 0 & \\
\theta_x(0,t) = -1 & t \geq 0 &
\end{array}
$$

It has been reported (G. Wilks and R. Hunt, *A finite time singularity of the boundary layer equations of natural convection*, ZAMP **36**(1985) 905–911) that computations show that solutions of this system (which arises in certain thermal convection problems) are never global in time. We have shown that there are no nontrivial stationary solutions and are working on the finite time blow up question. (A related problem was considered by C. I. Simpson and K. Stewartson in ZAMP(1982) 370-378. In that paper θ^2 replaces θ in the first equation and $\theta_x(0,t) = 1$.)

(Sacks)

1. The Inverse Dirichlet Problem. Consider the Sturm-Liouville problem

$$
\begin{array}{ll}
\varphi'' + (\lambda - q(x))\varphi = 0 & 0 < x < 1 \\
\varphi(0) = \varphi(1) = 0 &
\end{array}
$$

with $q \in L^2(0,1)$. It is known that the potential $q(x)$ is uniquely determined by the spectral data $\{\lambda_k, \rho_k\}$ where λ_k is the k'th eigenvalue and $\rho_k = \left(\varphi_k'(0)^2/\|\varphi_k\|^2\right)$, φ_k being the k'th eigenfunction. We have developed an interative solution procedure whose main ingredient is the solution of a certain Goursat problem at each step. This approach may involve considerably less computational effort than other methods, e.g. solving a Gelfand-Levitan integral equation. We have proved a theorem concerning the convergence of the successive iterates, and numerical examples seem to show that the method works quite well in typical cases.

Currently we are trying to adapt this technique to 4th order spectral roblems, e.g. the inverse problem for the Euler-Bernoulli beam.

2. The Mesa Problem. Consider the Cauchy problem for the porous medium equation,

$$u_t = \Delta u^m \qquad x \in R^n, \qquad t > 0$$
$$u(x,0) = f(x)$$

For any $m > 0$ and $f \in L^1(R^n)$ there exists a (weak) solution $u = u_m(x,t)$. We are interested in the following question. Does $\lim u_m(x,t)$ exist for fixed f, and if so, what is the limit? This question was first studeid by Elliott, Herrero, King and Ockendon, who did some asymptotic analysis and made some conjectures. We have proved rigorous results confirming these conjectures in some cases, extending earlier work of Caffarelli and Friedman. In all cases for which the answer is known, it may be described as follows. The limit is a function $u = u_\infty(x)$ where $u = f + \Delta w$, and $w = v - \psi$ where $\Delta\psi = f - 1$ and v satisfies the obstacle problem on R^n with obstacle ψ.

We have proved a similar result for the case that the space domain isn an interval in $\mathbf{R}$, with u satisfying zero boundary conditions. The case of a general bounded domain in R^n remains open.

3. Coefficient identification problem involving an unknown source. Consider a constant density acoustic half space $\{(x,y,z) : z \geq 0\}$ characterized by a sound speed $c(x,z) > 0$. At each point $(x_s,0,0)$ a source $f(t,x_s)$ of acoustic waves is set off, and the resulting reflected waves are measured at receiver location $x = x_s + h$ for some offset $h > 0$. Assuming that c is close to constant and $f(t,x_s)$ is close to some known impulsive wavelet $f_0(t,x_s)$ we show that $c - 1$ and $f - f_0$ can be uniquely recovered, in the linear approximation, from the surface reflection data at any two offsets, and all source locations $(x_s,0,0)$. A numerical method for this purpose is also discussed.

(Alexander)

1. Implicit Runge-Kutta Methods.

a) Higher order DIRK formulae. We have determined coefficients satisfying the algebraic identities required for a formula to be

- of order 4 or 5,
- diagonally implicit, that is, the coefficient matrix is lower triangular and all diagonal entries are equal,
- A-stable, so that the formula is possibly useful for solving stiff problems, and
- strongly S-stable, which is a consequence of the preceding two properties if the last quadrature point is 1 and the last row of the amtrix is the vector of quadrature weights.

We use numerical optimization in the solution variety to minimize the sum of squares of errors in the coefficients of differentials in the truncation error, subject to bounds on the coefficients. We have identified an optimal 4th order formula. Work on 5th order formulae is in progress.

b) The code DIRK based on these formulae is being prepared for submission to Transactions on Mathematical Software. This is an initial-value code with an adaptive equation-solving strategy suitable for both stiff and nonstiff problems; it uses Hermite quintic interpolation to provide dense output if required, without interfering with the optimally chosen stepsize.

c) We are studying the stability and error analysis of implicit Runge-Kutta formulae for the class of linear time-varying ODE systems with coefficient matrices essentially negative dominant in the sense of Kreiss. We seek to establish criteria for stability, and to show convergence to smooth solutions.

d) In collaboration with Ph.D. student J. J. Coyle, we have applied these methods to differential- algebraic systems. In work to appear in SIAM J. Numer. Analysis, we show how to overcome "order reduction", the observed loss of order of convergence of DIRK formulae. We derive conditions for the order of accuracy without assuming that the coefficient matrix is nonsingular, and establish algebraic conditions for a method with singular coefficient matrix to be well defined for linear constant-coefficient systems of arbitrary index. We present an example of a formula which converges with the desired order of accuracy on index-two systems on which Petzold's code DDASSL grinds to a halt.

2. Diffusion Flame in a Chamber.

Matalon, Ludford and Buckmaster derived the following boundary value problem in their study of the near-ignition regime for a diffusion flame in a chamber:

$$y'' + Qx^{-1}(1-x)e^{y} = 0, \qquad 0 < x < 1;$$
$$y(0) = y(0) = 0.$$

Numerical computation exhibit a value of $Q = Q^* > 0$ such that

there is no solution of the problem when $Q > Q^*$,

there is exactly one solution when $Q = Q^*$,

there are just two solutions when $0 < Q < Q^*$.

The analysis is interesting because of the singularity at $x = 0$. By formulating the problem in an appropriate function space and using the theory of monotone operators, we can demonstrate the first two properties and give upper and lower bounds on Q^*. We can show that there are at least two solutions for $0 < Q < Q^*$; it is expected that analysis of the eigenvalue problem for the linearized problem will yield the remaining part of the conclusion.

3. Two-Dimensional Digital Filter Stability.

A two-dimensional, linear shift invariant, quarter-plane causal digital filter is characterized by the z-transform of its impulse response, which is a rational function of two variables, say P/Q the zero sets of P and Q are algebraic curves in $2-D$, not isolated poles. It is a difficult problem to determine whether the filter is (BIBO-) stable when P

and Q, though relatively prime, have a common zero on the distinguished boundary of the unit bidisc, that is, on the torus.

Alexander and Woods (IEEE Trans. CAS, Sept. 1982) gave an analytical criterion in terms of absolute integrability of partial derivatives of the transform function. Dautov (USSR) has given an algebraic criterion when the denominator Q splits into linear factors.

We have reformulated Dautov's result in terms of the intersection number of the algebraic curves $P = 0$ and $Q = 0$ at the point of indeterminacy. We conjecture that this purely algebraic criterion suffices in general. A proof requires formulating the analytic consequences of this fact and showing that they are sufficient for absolute convergence of a double Fourier series.

4. Tubular Chemical Reactors.

Our recent study [SIAM J. Math. Anal., to appear] of the low conversion steady states improved the results of Alexander, [J. Math. Anal. Appl. June, 1984] in two respects:

We used the method of averaging to get an accurate count of the number of steady states;

We showed that the solutions of the approximating equation studied in the earlier paper actually yield solutions of the full reactor equations.

The late Professor Ludford asked whether any of these solutions were stable. We are now studying this problem. We also intend to use the AUTO code of Doedel to compute branches of time-periodic solutions originating at Hopf bifurcation points.

5. A Semilinear Wave Equation.

In our study of the problem

$$u_{tt} - u_{xx} = u^3 \cos u, \qquad 0 < x < 1, \qquad t > 0;$$
$$u(0,t) = u(1,t) = 0; \qquad u(x,0), u_t(x,0) \quad \text{given.}$$

we have computed a number of steady state solutions. LInearization about these steady states has revealed either all imaginary eigenvalues, or one pair of real eigenvalues (one positive and the other negative) with the remaining eigenvalues pure imaginary. (The spectrum has been computed numerically.) We shall look at solutions in the neighborhood of the "linearly neutrally stable" steady states in an attempt to detect the presence of a potential well. The multiplicity and structure of steady states seem to be accessible to analytical methods.

III. Completed Work (Papers in Preparation or Submitted).

A. H. A. Levine

1. (With C. Bandle) *On the existence and nonexistence of solutions of reaction-diffusion equations in sectorial domains,* Transactions of American Mathematical Society, (in print).

2. *Quenching, nonquenching and beyond quenching for solutions of some parabolic equations.* Annali di Mat. Pura et Applicada (in print).

3. (With P. Meier) *The value of the critical exponent for reaction-diffusion equations in cones,* Arch. Rat. Mech. Anal. (in print).

4. *The long time behavior of solutions of reaction-diffusion equations in unbounded domains: a survey,* Proceedings of 10th Dundee Conference on the Theory of Ordinary and Partial Differential Equations (in print).

5. (with Keng Deng) *On the blowup of u_t at quenching,* Proc. Am. Math. Soc. (in print).

6. (With R. Quintanilla) *Some remarks on Saint-Venant's Principle,* Math. Meth. Appl. Sci. (in print).

B. P. E. Sacks

1. *An iterative method for the inverse Dirichlet problem,* Inverse Problems, 4, 1988, 1055–1069.

2. *A singular limit problem for the porous medium equation,* to appear in J. Math. Anal. Appl.

3. *Some linearized inverse problems for acoustic media,* Proceedings of the 26th IEEE Conference on Decision and Control, 1987, 175–177.

4. (With W. Symes) *Velocity inversion from common offset data,* to appear in Inverse Problems.

5. *A velocity inversion problem involving an unknown source,* submitted to SIAM J. Appl. Math.

C. R. K. Alexander

1. *Spatially oscillatory steady states of tubular chemical reactors,* SIAM J. Math. Anal. (in print).

2. *A DIRK for all seasons,* to be submitted to ACM TOMS.

3. (with J. J. Coyle) *Runge-Kutta methods and differential-algebraic systems,* SIAM J. Num. Anal. (in print).

IV. Personnel.

A. Senior Personnel (with period of support)

1. Professor Howard A. Levine, P.I. (June, July 1988)

2. Associate Professor Paul E. Sacks (June, July 1988)

3. Associate Professor Roger K. Alexander (June, July 1988)

B. Graduate Research Assistants

1. Jeffrey Anderson (Ph.D. Candidate) will finish 5/20/89.

2. Sang Ro Park (Ph.D. Candidate) will finish 5/20/89.

3. Keng Deng (Ph.D. Candidate) will finish 12/18/89.

4. Kurugamega Jayawardena (Ph.D. Candidate)

5. James Coyle (Ph.D. Candidate)

V. Interactions (supported in part by AFOSR 88-0031).

A. H. A. Levine

1. Visited Cornell University and consulted with L. E. Payne on some problems in convective heat conduction. 3/11/88-3/18/88.

2. Consulted with C. Bandle on blow up for reaction-diffusion equations, Basel, Switzerland. 5/30/89 to 6/12/89. (Overseas airfair paid by the Swiss N.S.F.)

3. Gave a plenary lecture at the Tenth Dundee Conference on Differential Equations on reaction diffusion equations at the University of Dundee 7/5/88 to 7/9/88

4. Attended CBMS conference on Nonlinear Wave Equations to be given at George Mason University 1/16/89–1/20/89.

B. P. E. Sacks

1. Attended 26th IEEE Conference on Decision and Control, Los Angeles, 12/9/87–12/11/87, and gave lecture 'Some linearized inverse problems for acoustic media'.

2. Attended AMS national meeting, Atlanta, 1/6/88–1/9/88, and gave talk in special session, 'The inverse problem for a weakly inhomogeneous two dimensional acoustic medium'.

3. Attended A.M.S. regional meeting, East Lansing 3/18/88–3/19/88, and gave talk in special session, 'A singular limit problem for the porous medium equation'.

4. Attended MIPAC Workshop on Computational and Experimental Aspects of Control, Madison, 5/16/88–5/18/88.

5. Attended NSF-CBMS research conference on Weak Convergence Methods in Nonlinear Partial Differential Equations, Loyola Univ., 6/27/88–7/1/88.

6. Visited Rice University, 6/11/88–6/15/88, consulted with W. Symes.

7. Visited Rice University, 1/26/89–1/29/89, consulted with W. Symes.

C. R. K. Alexander

1. Attended AFOSR Contractors' Meeting on Combustion, University Park, Pennsylvania, 6/21/87–6/24/87

2. Attended Numerical ODE Conference, Toronto, 6/20/88–6/22/88.

3. Attended SIAM National Meeting in Minneapolis, Minnesota, 7/11/88–7/15/88, and presented the paper *The Runge-Kutta method and differential-algebraic equations*, (joint with J. Coyle).